Indian J. Phys. **52B**, 410–415 (1978)

On superposition of Kratzer and a general potential

S. S. RAGHUWANSHI AND L. K. SHARMA

Department of Applied Physics, Government Engineering College, Jabalpur-482011

(*Received* 20 *September* 1977, *revised* 21 *February* 1978)

Large coupling expansion of eigenenergies of a potential which is the superposition of Kratzer's molecular and a general potential has been obtained. The utility of this superposed potential has also been discussed.

1. INTRODUCTION

Recently there has been a considerable revival of interest in the analytic properties of scattering amplitudes in the frame of quantum mechanics and potential theory. This interest is largely due to the fact that in potential theory many problems are solvable either exactly or else approximately by well-known methods, whereas fully relativistic theories often lead to insurmountable mathematical difficulties. Large coupling expansions of eigenenergies have attracted considerable interest recently in particle physics with a view to understand strong interactions in terms of field-theoretic formulations.

There are only few large coupling constant field theoretical models. They have recently been studied by Cheng & Wu (1973). In the frame of quark model they have been studied by Joos & Krammer (1971). Large coupling solutions of the Bethe-Salpeter equation in the frame of Wick-Cutkosky model have been discussed by Müller (1972). Non-relativistic Schrödinger equation for large coupling constants for the Gauss (1970) and the generalized Yukawa potential (1973) have been studied. Large coupling constants expansions of the eigenenergies for a general even power potential (1971) and the superposition of inverse square and Yukawa potentials (1977) have also been obtained.

In the present paper, the superposition of Kratzer's molecular and a general potential has been considered. In section 2, the eigenenergy expansion of the superposed potential has been derived. In section 3, a brief discussion on the practical application of the superposed potential in molecular physics is mentioned.

2. EGIENENERGIES

We consider the radial Schrödinger equation,

$$\left[\frac{d^2}{dr^2}+k^2-\frac{l(l+1)}{r^2}-V(r)\right]\psi(r)=0 \qquad \ldots\ (2.1)$$

$\hbar = c = 1$, $m = \frac{1}{2}$ for a potential which is the superposition of Kratzer molecular and a general potential of the form

$$V(r) = -2D\left(\frac{a'}{r} - \frac{1}{2}\frac{a'^2}{r^2}\right) - D\left\{\sum_{i=0}^{\infty} \alpha^i N_i r^i\right\} \qquad \ldots (2.2)$$

(Kratzer) (General)

In the limit $\alpha \to 0$, potential (2.2) reduces to

$$V(r) = -2D\left(\frac{a'}{r} - \frac{1}{2}\frac{a'^2}{r^2}\right) - DN_0 \qquad \ldots (2.3)$$

Setting $k^2 = E$, $x = r/a'$, $\beta^2 = -a'^2E$, $\beta'^2 = \beta^2 - \gamma^2 N_0$, $\gamma^2 = a'^2D$ transforms (2.1) with potential (2.3) as

$$\frac{d^2\psi}{dx^2} + \left[-\beta'^2 + \frac{2\gamma^2}{x} - \frac{\gamma^2 + l(l+1)}{x^2}\right]\psi = 0. \qquad \ldots (2.4)$$

Further setting

$$\psi = x^\lambda e^{-\beta' x}\phi(x) \qquad \ldots (2.5)$$

where

$$\lambda = \tfrac{1}{2} + \sqrt{\gamma^2 + (l+\tfrac{1}{2})^2}, \qquad (\lambda > 1) \qquad \ldots (2.6)$$

transforms (2.4) to the confluent hypergeometric equation whose solution for bound states ($\beta' > 0$) has the form :

$$\psi = x^\lambda e^{-\beta' x}\,{}_1F_1(\lambda - \gamma^2/\beta',\ 2\lambda;\ 2\beta' x) \qquad \ldots (2.7)$$

Taking

$$\lambda - \gamma^2/\beta' = a = -n,\ n = 0, 1, 2, \ldots \qquad \ldots (2.8)$$

Eq. (2.8) yields the energy levels as

$$E = k^2 = -\gamma^4/a'^2(n+\lambda)^2 - DN_0. \qquad \ldots (2.9)$$

Therefore, in the general case we may write

$$k^2 = \frac{-\gamma^4}{a'^2(n+\lambda)^2} - DN_0 + D\Delta. \qquad \ldots (2.10)$$

Writing for k^2 from (2.10) in the radial Schrödinger equation with the general potential (2.2) one gets

$$D_n\psi = -D\Delta\psi - D\left\{\sum_{i=0}^{\infty} \alpha^i N_i r^i \psi\right\} \qquad \ldots (2.11)$$

where,

$$D_n \equiv \left[\frac{d^2}{dr^2} - \frac{\gamma^4}{a'^2(n+\lambda)^2} - DN_0 - \frac{l(l+1)}{r^2} + 2D\left(\frac{a'}{r} - \frac{1}{2}\frac{a'^2}{r^2}\right)\right] \qquad \ldots (2.12)$$

As a first approximation to ψ we have

$$\psi \simeq \psi^{(1)} = \psi_n(x) - x^{\lambda} e^{-\beta' x} {}_1F_1(\lambda - \gamma^2/\beta', 2\lambda; 2\beta' x). \quad \ldots (2.13)$$

This approximation obviously leaves uncompensated term on the right hand side of (2.14) amounting to

$$R^{(1)} = \left[-D\Delta - D\left\{ \sum_{i=0}^{\infty} \alpha^i N_i r^i \right\} \right] \psi. \quad \ldots (2.14)$$

Following Müller *et al* (1968), (2.14) can be solved by using the following recurrence relation of the confluent hypergeometric functions :

$$Z\psi(a) = (a, a+1)\psi(a+1) + (a, a)\psi(a) + (a, a-1)\psi(a-1) \quad \ldots (2.15)$$

where

$$\psi(a) = \psi(a, b; z) \quad \text{and} \quad z = 2\beta' x$$

$$(a+1, a) = a = -n$$

$$(a, a+1) = a - b + 1 = n - \frac{2\gamma^2}{\beta'} + \Delta + 1$$

$$(a, a) = (b - 2a) = \frac{2\gamma^2}{\beta'} - \Delta$$

$$(a, a+1) = a - 1 = -n - 1 \quad \ldots (2.16)$$

In general,

$$Z^m \psi(a) = \sum_{j=m}^{-m} S_m(a, j)\psi(a+j) \quad \ldots (2.17)$$

with coefficients S_m satisfying following recursion relation

$$S_m(a, r) = S_{m-1}(a, r+1)(a+r-1, a+r) + S_{m-1}(a, r)(a+r, a+r) + S_{m-1}(a, r+1)(a+r+1, a+r),$$

with boundary conditions as

(i) $S_0(a, 0) = 1$ and all $S_0(a, j \neq 0) = 0$

(ii) $S_m(a, r) = 0$ for $|r| > m$. $\quad \ldots (2.18)$

Eq. (2.14) with the help of (2.15)–(2.18) can be written as

$$R^{(1)} = D[a, a]_1 \psi(a) + D \sum_{i=1}^{\infty} (\alpha)^i \sum_{j=-1}^{i} [a, a+j]_{i+1} \psi(a+j) \quad \ldots (2.19)$$

where

$$[a, a]_1 = -\Delta + N_0$$

and

$$[a, a+j]_{i+1} = N_i S_i(a, j). \quad \ldots (2.20)$$

Next we observe that

$$D_n \psi(a+j) = j\psi(a+j). \quad \ldots (2.21)$$

Thus a term $(\alpha)^i[a, a+j]_{i+1}\psi(a+j)$ in (2.19) can be cancelled out by adding to the previous approximation the contribution

$$(\alpha)^i \frac{[a, a+j]_{i+1}}{j} \psi(a+j)$$

except of course, when $j = 0$. The next contribution to $\psi^{(1)}$ is therefore

$$\psi^{(2)} = \sum_{i=1}^{\infty} (\alpha)^i \sum_{\substack{j=-i \\ j\neq 0}}^{i} \frac{[a, a+j]_{i+1}}{j} \psi(a+j). \quad \ldots (2.22)$$

This process may be repeated indefinitely. Then adding successive contributions and rearranging them we obtain

$$\psi = \psi^{(1)} + \psi^{(2)} + \ldots.$$

Adopting the procedure of Müller *et al* (1968), the value of Δ given in eq. (2.10) can be written as

$$0 = [a, a]_1 + \alpha[a, a]_2 + \alpha^2[a, a]_3 + \alpha^3[a, a]_4 + \alpha^4 \left\{[a, a]_4 + \frac{[a, a+1]_2}{1}[a+1, a]_2 + \frac{[a, a-1]_2}{-1}[a-1, a]_2\right\} + O(\alpha^5). \quad \ldots (2.23)$$

This is the equation from which Δ and hence the eigeneregy k^2 is determined. Evaluation yields the expansion

$$\frac{1}{D}\left[k^2 + \frac{\gamma^4}{a'^2(n+\lambda)^2}\right] = -\alpha N_1\left[\frac{2\gamma^2}{\beta'} + N_0\right] - \alpha^2\left[\{-N_1^2 N_0 - N_2 N_0^2 + 2N_2 n(n+1) + N_2 N_0(n+1) + N_2 N_0 n\} + \left(\frac{2\gamma^2}{\beta'}\right) \times \{N_1^2 + 2N_0 N_2 - N_2 n - N_2(n+1)\} - N_2\left(\frac{2\gamma}{\beta'}\right)^2\right] + O(\alpha^3). \quad \ldots (2.24)$$

This is the general eigenenergy expansion for the superposition of Kratzer and the general potentials. Putting coefficients (N_i) equal to zero in (2.2), the general potential is reduced to Kratzer molecular potential. Thus the eigenenergy expansion for Kratzer potential is obtained from (2.24) as :

$$k^2 = -\frac{\gamma^4}{a'^2(n+\lambda)^2}. \quad \ldots (2.25)$$

Similarly for $a' = 0$ ($\gamma = a'D^{\frac{1}{2}} = 0$), the potential (2.2) is reduced to the general potential $V(r) = D\sum_{i=0}^{\infty} \alpha^i N_i r^i$ and the eigenenergy expression for this potential has the form

$$k^2 = -D\alpha N_1 N_0 - D\alpha^2\{-N_1^2 N_0 + \ldots\} + O(\alpha^3). \quad \ldots (2.26)$$

3. Conclusion

The potential given in eq. (2.2) may be taken as the superposition of Kratzer's molecular potential and the Morse potential. Obviously this potential satisfies fully the criteria formulated by Varshni (1957) for being a suitable function for diatomic molecules. Detailed study of this potential from the point of view of its application in molecular physics has been made by us and the results so obtained are to be published elsewhere.

In this investigation, binding energies of all angular momenta for potential (2.2) in the form of an asymptotic expansion has been obtained. The method used by us, as has already been discussed in detail (1977) is quite useful and can be applied in solving a few other problems of importance.

The eigenvaludes of Kratzer and the superposed potential have been plotted in figure 1, for different quantum states. The energy levels always lie lower

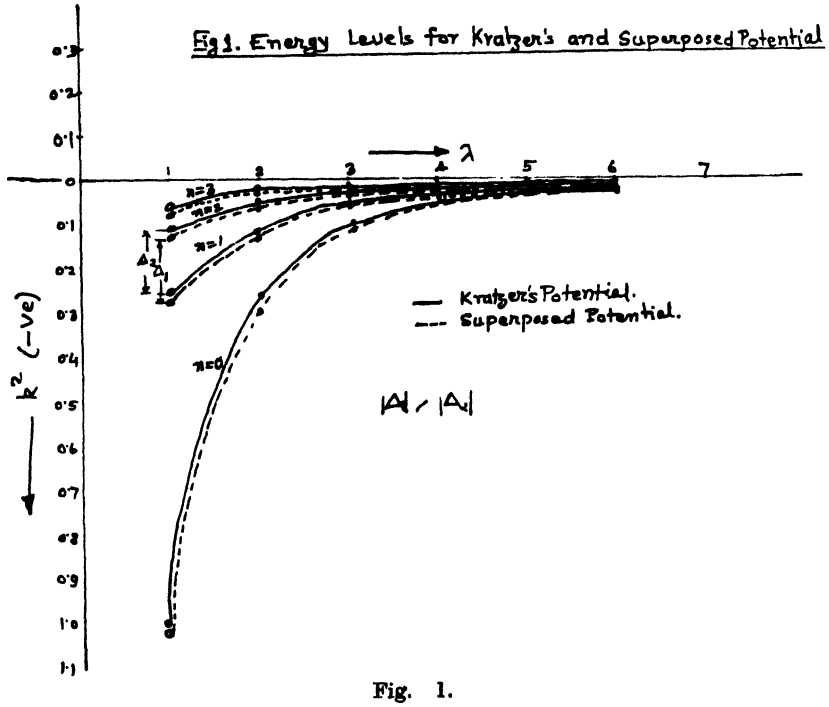

Fig. 1.

in the superposed potential considered in this paper than for the Kratzer potential. Further, it may be of interest to note the following :—

(i) The crowding together of the upper levels for Kratzer potential is more rapid than that for the superposed potential.

(ii) The energy levels for both the superposed potential and the Kratzer potential lie in the negative energy region. The energy levels of the superposed

potential always lie below the energy levels for the Kratzer potential lone. This clearly indicates that the binding in the case of the potential (2.2) is stronger than for the Kratzer potential. The shift in energy levels of superposed potential is obviously due to the perturbation of general potential $\left[V(r) = -\sum_{i=0}^{\infty} \alpha^i N_i r^i\right]$ over the Kratzer's molecular potential.

ACKNOWLEDGMENT

The authors are grateful to Dr. M. C. Sen for the encouragement. One of the authors (S.S.R.) is grateful to C.S.I.R., India for the award of Junior Fellowship.

REFERENCES

Cheng H. & Wu T. T. 1973 *Phys. Rev.* **D8**, 450.

Joos H. & Krammer M. 1971 *Nuovo Cim.*

Müller H. J. W. 1972 *Nuovo Cim.* **10A**, 76.

Müller H. J. W. 1970 *J. Math. Phys.* **11**, 355.

Müller H. J. W. & Faridi N. Vahedi 1973 *J. Math. Phys.* **14**, 1291.

Müller H. J. W. & Schilcher K. 1968 *J. Math. Phys.* **9**, 255.

Raghuwanshi S. S. & Sharma L. K. 1977 *Large coupling expansions for eigenenergies of superposition of Inverse square and Yukawa potentials (to be published in the Indian Journal of Physics).*

Sharma L. K. 1971 *Ph.D. thesis A.P.S. University, Rewa, India* (unpublished).

Varshni Y. P. 1957 *Rev. Mod. Phys.* **29**, 664.